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Atomic data from the iron project

LXI. Radiative E1, E2, E3, and M1 transition probabilities for Fe IV⋆

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ABSTRACT

Radiative decay rates (A) and line strengths (S) are presented for a large number of electric dipole allowed (E1) and forbidden electric quadrupole (E2), octupole (E3) and magnetic dipole (M1) transitions in Fe IV. The ion is amongst the most complex iron ions and exhibits effects of strong electron correlation. It has closely spaced fine structure levels from seven configurations: $3s^23p^63d^5$, $3s^23p^63d^44s$, $3s^23p^63d^44p$, $3s^23p^63d^44d$, $3s^23p^63d^34s4p$, $3s^23p^63d^34s4d$, $3s^23p^53d^6$ before an energy gap could be noted. Atomic parameters are presented for multipole radiative transitions among the 1275 fine structure levels dominated by these seven configurations. A total of approximately 173 000 transitions of type E1, E2, E3 and M1 are presented, The set of intercombination and forbidden transitions complements the earlier extensive set of dipole allowed ($\Delta J = 0, \pm1$, $\Delta L = 0, \pm1$, and $\Delta S = 0$) fine structure transitions in Fe IV. The results are obtained in the relativistic Breit-Pauli approximation using an updated atomic structure code SUPERSTRUCTURE. Transition probabilities are compared with the existing results and varying degrees of agreement are found. The total number of transitions presented should provide a reasonably complete set for modeling of most optical to ultraviolet Fe IV spectra of astrophysical sources.

Key words. atomic data – line: formation – radiation mechanisms: general – atomic processes

1. Introduction

The low ionization stages of iron are of importance in astronomy due to the multitude of transitions across multi-wavelength regions of the electromagnetic spectrum observed from a wide variety of astrophysical objects, such as nebulae (e.g. Pequignot & Baluteau 1994; Kwok 2003), stars (e.g. Werner et al. 2003; Lanz & Hubeny 2003), active galactic nuclei (e.g. Sigut & Pradhan 2003; Rodríguez-Ardila 2002) etc. However, the atomic physics of these heavy, many-electon systems is complicated and several important physical effects must be considered in theoretical computations. Fe IV is of particular interest for astrophysical plasmas since its ionization potential ∼54.8 eV is close to that of He II at 54.4 eV, causing the main sequence O and B stars to have a 54 eV "cut-off" which attenuates the ionizing flux. Forbidden lines of Fe IV were detected in the Orion Nebula (Rubin et al. 1997) and other nebulae (Rodriguez 2003). The luminosity of an emission line gives a measure of the temperature and other physical conditions of the plasmas. Accurate parameters for a large number of atomic radiative transitions are needed for a wide range of applications, from diagnostics of specific spectral features to calculations of plasma opacities in stellar and non-stellar astronomical objects. The present set of A-values for the forbidden transitions should be useful for such needs.

Fe IV is one of the computationally most challenging iron ions. The complexity arises from configurations of half or nearly half-filled 3d shells with additional 4l electrons. The calculated spectrum gives rise to a large number of almost continuous energy levels, as noted in our earlier work (Nahar & Pradhan 2005). An extensive set of fine structure dipole allowed transitions was presented in that work where results were obtained using close coupling R-matrix method. However, very limited account was taken of relativistic effects, including only the one-body mass correction and Darwin terms. The dipole allowed same-spin-multiplet transitions generally represent the strongest lines in an atom or ion. The earlier calculations included a large set of such $\Delta S = 0$ transitions among all bound levels with $n \leq 11$ and $l \leq (n-1)$. The intercombination and forbidden lines are usually visible for low lying excited states. The present results include intercombination E1 ($\Delta S \neq 0$) and forbidden E2, E3 and M1 transitions, and thus complement and complete the earlier dataset.

2. Theory

Present line strengths and radiative decay rates for the allowed and forbidden transition in Fe IV are obtained in a

⋆ Complete electronic data tables of energies and transition probabilities are available from the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/448/779

configuration interaction atomic structure calculation, as was employed for Fe XVII (Nahar et al. 2003) and Fe XX (Nahar 2003). Relativistic effects are included through the Breit-Pauli approximation in the updated version of the atomic structure code SUPERSTRUCTURE (Eissner et al. 1974) extended to include higher order multipole transitions, E2, E3, M1, M2. Theoretical details of the method can be found in Eissner (1991), Eissner & Zeippen (1981) and Nahar et al. (2003). A brief description of the theory is given below.

In non-relativistic atomic structure calculations, the energies and wavefunctions of an N-electron ion are obtained through optimum solutions of the Schrodinger equation,

$$\left[\sum_{i=1}^{N}\left\{-\nabla_i^2-\frac{2Z}{r_i}+\sum_{j>i}^{N}\frac{2}{r_{ij}}\right\}\right]\Psi = E\Psi, \tag{1}$$

where $\Psi = \Psi(\gamma S L M_S M_L|\boldsymbol{r}_1, ..., \boldsymbol{r}_N)$ are the bound solutions consisting of a linear combination of configuration state functions. The antisymmetrization is carried out by expansion of products of single particle wavefunctions. The present approximation represents the nuclear and electron-electron potential by a statistical (Thomas-Fermi-Dirac-Amaldi) model potential $V^{SM}(r) = \frac{Z_{\rm eff}(\lambda_{nl},r)}{r}$ where $Z_{\rm eff}(\lambda_{nl}, r) = Z[{\rm e}^{-Zr/2} + \lambda_{nl}(1-{\rm e}^{-Zr/2})]$ and λ_{nl} are the Thomas-Fermi scaling parameters for each orbital.

The relativistic N-electron Hamiltonian in the Breit-Pauli (BP) approximation is (e.g. Eissner 1991)

$$H_{\rm BP} = H_{\rm NR} + H_{\rm mass} + H_{\rm Dar} + H_{\rm so}$$
$$+\frac{1}{2}\sum_{i\neq j}^{N}\Big[g_{ij}\,(so+so')+g_{ij}\,(ss')+g_{ij}\,(css')+g_{ij}(d)+g_{ij}\,(oo')\Big]. \tag{2}$$

$H_{\rm NR}$ is the non-relativistic Hamiltonian, and

$$H_{\rm mass} = -\frac{\alpha^2}{4}\sum_i p_i^4, \qquad H_{\rm Dar} = -\frac{\alpha^2}{4}\sum_i \nabla^2\left(\frac{Z}{r_i}\right),$$
$$H_{\rm so} = \alpha^2\sum_{i=1}\frac{Z}{r_i^3}{\rm l}(i)\cdot{\rm s}(i) \tag{3}$$

are the relativistic one-body mass correction, Darwin, and spin-orbit interaction terms. The rest are two-body interaction terms with notation c for contraction, d for Darwin, o for orbit, s for spin and a prime indicates "other". The present approximation ignores the last three two-body terms, but includes the contribution of the full Breit interaction term consisting of the fine structure terms, that is spin-other-orbit (os') and spin-other-spin (ss') terms,

$$H^B = \sum_{i>j}\Big[g_{ij}\,(so+so') + g_{ij}\,(ss')\Big], \tag{4}$$

where

$$g_{ij}\,(so+so') = -\alpha^2\left(\frac{\boldsymbol{r}_{ij}}{r_{ij}^3}\times\boldsymbol{p}_i\right).\left(\boldsymbol{s}_i+2\boldsymbol{s}_j\right)+\left(\frac{\boldsymbol{r}_{ij}}{r_{ij}^3}\times\boldsymbol{p}_j\right).\left(\boldsymbol{s}_j+2\boldsymbol{s}_i\right),$$
$$g_{ij}\,(ss') = 2\alpha^2\frac{\boldsymbol{s}_i.\boldsymbol{s}_j}{r_{ij}^3} - 3\frac{\left(\boldsymbol{s}_i.\boldsymbol{r}_{ij}\right)\left(\boldsymbol{s}_j.\boldsymbol{r}_{ij}\right)}{r_{ij}^5}. \tag{5}$$

The electron–electron correlations contribute dominantly through *1/Z* dependence while the relativistic corrections play an important role in the distribution of fine structure components for weaker transitions. The one-body terms vary as α^2Z^4 and contribute in general more than the two-body terms with one less power of Z.

The primary quantity expressing radiative excitation or de-excitation is the line strength (Nahar et al. 2003)

$$S^{X\lambda}(ij) = \left|\left\langle\Psi_j\right\|O^{X\lambda}\left\|\Psi_i\right\rangle\right|^2, \qquad S(ji) = S(ij). \tag{6}$$

where X denotes the type, electric or magnetic, and λ denotes the order of multipoles of operator O. $S^{X\lambda}(ij)$ does not explicitly depend on the transition energy for *electric* multipole transitions in the length formulation since

$$O^{{\rm E}\lambda} = b^{[\lambda]}\sum_{p=1}^{N}{\rm C}^{[\lambda]}(p)r_p^{\lambda}, \qquad b^{[\lambda]} = \sqrt{\frac{2}{\lambda+1}}. \tag{7}$$

For the case of electric dipole radiation, Eλ = E1. Electric dipole allowed E1 transitions ($\Delta J = 0, \pm 1$, parity (π) changes, that is, odd parity $\leftrightharpoons$ even parity) include both allowed same-spin-multiplets ($\Delta L = 0, \pm1, \pm2$, $\Delta S = 0$) and intercombination ($\Delta L = 0, \pm1 \pm 2$, $\Delta S \neq 0$) transitions. Transition probabilities or Einstein's coefficient for radiative decay rates (A-values) and *absorption* oscillator strengths (f-values) for transitions between levels i and j for E1 transitions are written in terms of the line strength S as

$$f_{ij} = \frac{E_{ji}}{3g_i}S^{\rm E1}(ij), \quad g_i f_{ij} = -g_j f_{ji} = (gf)_{ij} \tag{8}$$

$$A_{ji}^{\rm E1}\cdot\tau_0 = \alpha^3\frac{g_i}{g_j}E_{ji}^2 f_{ij} \tag{9}$$

where the scaling of energies is in units of Ry = $\frac{\alpha^2}{2}m_{\rm el}c^2$ = 13.6 eV, and the time unit is $\tau_0 = \hbar/{\rm Ry} = 4.838\times10^{-17}\cdot$ s: $E_{ij} = E_j - E_i$ is the excitation energy, g_j and g_i are the statistical weights of the upper and lower states respectively, and α is the fine structure constant.

In the magnetic dipole (M1) case the radiative operator for the line strength expression (6) reads

$$O^{\rm M1} = \sum_p {\rm l}(p) + 2{\rm s}(p) + \frac{\alpha^2}{2}\left\{\frac{\partial^2}{\partial r_p^2}+\ldots+\sum_{p'>p}\frac{\ldots}{r_{p'p}}\right\}; \tag{10}$$

where the sum runs over electron coordinates, l and s are the orbital and spin operators respectively. Details of the correction of relative BP order can be found in Eissner & Zeippen (1981).

For the forbidden electric quadrupole (E2) and the magnetic dipole (M1) transitions ($\Delta J = \pm0, 1, 2$ and parity remains unchanged) the radiative decay rates, A(E2) and A(M1), are given by:

$$A_{ji}^{E2} = 2.6733\times10^3\left(E_j-E_i\right)^5/g_jS^{E2}(i,j)\ {\rm s}^{-1}, \tag{11}$$

$$A_{ji}^{M1} = 3.5644\times10^4\left(E_j-E_i\right)^3/g_jS^{M1}(i,j)\ {\rm s}^{-1}, \tag{12}$$

and for the electric octopole (E3) transition ($\Delta J = \pm2, \pm3$ and even parity $\leftrightarrow$ odd parity) the radiative decay rates A(E3) are given by:

$$A_{ji}^{\rm E3} = 1.2050\times10^{-3}\left(E_j-E_i\right)^7/g_jS^{\rm E3}(i,j)\ {\rm s}^{-1}, \tag{13}$$

where $E_j > E_i$ (the energies are in Rydbergs), and $\mathcal{S}$ is the line strength for the corresponding transition.

The lifetime of a level can be computed as

$$\tau_k = \frac{1}{\sum_i A_{ki}}, \quad (14)$$

where the sum is the total radiative transition probability for level k. A Fortran program (LIFETMBP) is provided to compute the lifetime of any level from the given set of A-values.

3. Atomic calculations

Fe IV computationally had been a challenging ion: the extended version of SUPERSTRUCTURE (Nahar et al. 2003) required about 7–10 CPU hours of the supercomputer Cray SV1 for a trial run to determine a reasonable basis set of dominant configurations for the wavefunction expansion. It was necessary to include a set of excited configurations as their interactions introduced many closely lying energy levels. A set usually can be determind after an energy gap has been found indicating weakening interaction. Such a set for Fe IV is obtained by optimization over the lowest 474 LS terms of 7 configurations, $3s^23p^63d^5$, $3s^23p^63d^44s$, $3s^23p^63d^44p$, $3s^23p^63d^44d$, $3s^23p^63d^34s4p$, $3s^23p^53d^6$, and $3s^23p^63d^34s4d$. The scaling parameters λ_{nl} for the Thomas-Fermi-Dirac-Amaldi type potential of nl orbitals are 1.4(1s), 1.1128(2s), 1.27(2p), 1.27(3s), 1.073(3p), 1.058(3d), 1.073(4s), 1.06(4p), 1.008(4d).

Due to computational complexity and extended CPU time on the Cray SV1, E1 and E3 transitions were obtained separately from E2 and M1 transitions, and M2 transitions were omitted. E2 and M1 transitions were considered with the even parity configurations only. The transitions among the very high lying levels were not obtained. These transitions are not expected to contribute much to astrophysical models as most of the intercombination and forbidden transitions are weak, especially among the high lying ones.

The level energies are measured more accurately than the theoretical calculations. Hence, experimental energy level differences, wherever available, are employed in reprocessing of all types of transition probabilities (A-values) for improved accuracy. They are obtained from the energy independent line strengths. The processing of the large amount of data were carried out using coded PRCSS.

4. Results and discussion

Radiative decay rates (A-values) and line strengths (S) of about 173 000 transitions of type allowed E1 and forbidden E2, E3, M1 in Fe IV are presented. A total of 1275 fine structure levels were obtained from the seven lowest configurations. 269 of these levels have been observed. Both the table of energy levels and transition probabilities are available electronically.

A sample set of energies employed in the transitions is given in Table 1. The set is composed of a mixture of available observed energies (replacing the calculated ones) and the calculated ones for which no observed energies are available. As explained above, observed transition energies are implemented for improved accuracy. The measured energies by Ekberg & Edlen (1978) are available from the NIST (National Institute for Standards and Technology) database compiled by Sugar & Corliss (1985). The column $SL\pi(cf\#)$ in Table 1

Table 1. Sample set of fine structure energies employed in the transition probabilities for Fe IV. The number within parentheses next to each term correspond to configurations, $3s^23p^63d^5$(1), $3s^23p^63d^44s$(2), $3s^23p^63d^44p$(3), $3s^23p^63d^44d$(4), $3s^23p^63d^34s4p$(5), $3s^23p^53d^6$(6), $3s^23p^63d^34s4d$(7).

i	$SL\pi$(cf#)	2J	cfg	E(Ry)
1	6Se(1)	5	3d5	0.0000E+00
2	4Ge(1)	5	3d5	2.9435E-01
3	4Ge(1)	7	3d5	2.9439E-01
4	4Ge(1)	11	3d5	2.9384E-01
5	4Ge(1)	9	3d5	2.9427E-01
6	4Pe(1)	5	3d5	3.2126E-01
7	4Pe(1)	3	3d5	3.2198E-01
8	4Pe(1)	1	3d5	3.2265E-01
9	4De(1)	7	3d5	3.5338E-01
10	4De(1)	1	3d5	3.5445E-01
11	4De(1)	3	3d5	3.5483E-01
12	4De(1)	5	3d5	3.5480E-01
13	2Ie(1)	11	3d5	4.2901E-01
14	2Ie(1)	13	3d5	4.2912E-01
15	2Fe(1)	5	3d5 2	4.7538E-01
16	2De(1)	3	3d5 3	4.5610E-01
17	2Fe(1)	7	3d5 2	4.6834E-01
18	4Fe(1)	5	3d5	4.8150E-01
19	4Fe(1)	9	3d5	4.7952E-01
20	4Fe(1)	7	3d5	4.8020E-01
21	4Fe(1)	3	3d5	4.8149E-01
22	2De(1)	5	3d5 3	4.5146E-01
23	2He(1)	9	3d5	5.1084E-01
24	2He(1)	11	3d5	5.1367E-01
25	2Ge(1)	7	3d5 2	5.2314E-01
26	2Ge(1)	9	3d5 2	5.2599E-01
27	2Fe(1)	5	3d5 1	5.5730E-01
28	2Fe(1)	7	3d5 1	5.5819E-01
29	2Se(1)	1	3d5	6.0800E-01
30	2De(1)	3	3d5 2	6.7522E-01
31	2De(1)	5	3d5 2	6.7555E-01
32	2Ge(1)	9	3d5 1	7.5539E-01
33	2Ge(1)	7	3d5 1	7.5542E-01
34	6De(2)	1	3d4(5D)4s	1.1643E+00
35	6De(2)	3	3d4(5D)4s	1.1658E+00
36	6De(2)	5	3d4(5D)4s	1.1682E+00
37	6De(2)	7	3d4(5D)4s	1.1714E+00
38	6De(2)	9	3d4(5D)4s	1.1752E+00
39	2Pe(1)	3	3d5	9.1234E-01
40	2Pe(1)	1	3d5	9.1242E-01
41	2De(1)	5	3d5 1	9.8637E-01
42	2De(1)	3	3d5 1	9.8652E-01
43	4De(2)	1	3d4(5D)4s	1.2548E+00

specifies the LS term, $^{2S+1}L^{\pi}$, with configuration number within parentheses as numbered in the table caption. The next two columns give the value of $2J$ and configuration of the level. For an observed level, LS term of the core is specified following the table in the NIST compilation, However, it is not specified for a level with calculated energy since the level is identified by the energy eigenvalue with configuration of the core added by the valence electron. The last column in the table gives the relative energies in Rydberg unit.

The calculated energies are not optimized because of associated computational difficulties. There are differences between the calculated and observed energies although they narrow with higher levels. The difference is maximum for the lower levels of the ground configurations $3p^6 3d^5$, over 10%, but reduces to 5% or less for most of the levels of configuration 2 and a few to less than 1% for the 3rd excited configuration. This trend indicates that the difference will be much smaller for the levels of the rest of the excited configurations, numbered 4 to 7, for which no observed energies are available. It is often a trade off with a limited number of configurations to obtain more accurate energies for lower levels and larger uncertainty for higher levels and vice versa. Nonetheless, there is a room for improvement for the energy dependent f and A-values for which accurate transition energies are available, as implemented here. This technique, introduced by NIST, has been used for other ions, for example, by Nahar for Fe II (1995), by Nahar & Pradhan for Fe III (1996) etc., and by Froese Fischer & Rubin (2004) for the present ion, Fe IV.

A total of 44836 transition probabilities for electric dipole allowed E1 transitions of Fe IV are obtained. Sample sets are presented in Table 2. The E1 transitions include both the same-spin and the mixed-spin (intercombination) transitions. We present the "length form" A-values for the transitions as these are obtained more accurately than the "velocity form" values. The velocity form f-values are obtained only for E1 transitions where the difference between the length and velocity forms show very good to fair agreement, and relatively large differences for some transitions. The agreement between the two forms is not a sufficient criterion for the accuracy of the A or f values since wavefunctions of varying accuracies can be generated from various approximations. While A-values obtained from the central field approximation, which excludes most of the effects of a multielectron system, can be far away but often show very good agreement between the two forms. On the other hand wavefunctions including configuration interactions can yield more accurate A-values, but may not show the same agreement between the two forms.

About one third of the E1 transitions, 14 145, are of same-spin type with $\Delta L = 0, \pm 1$. These transitions were obtained earlier by Nahar & Pradhan (2005) but using the R-matrix method. A comparison is made of the two sets of dipole allowed same-spin transitions in Table 3 with good agreement in general, such as for $a^6\mathrm{S} - z^6\mathrm{P}^{\circ}$. Differences larger than 10% are also seen, for example for $a^6\mathrm{D} - z^6\mathrm{F}^{\circ}$. The earlier R-matrix close coupling calculations represent a better configuration interaction for the electron-electron correlation and could be preferable for stronger transitions and the present atomic structure calculations consider the relativistic effects more accurately and

Table 2. Samples of line strengths S and radiative decay rates or Einstein's A-coefficients for the allowed E1 (both same-spin and intercombination), forbidden electric quadrupole (E2), octupole (E3) and magnetic dipole (M1) transitions in Fe IV. N is the level number, TC are the LS term and configuration number (see Table 1) and g is the statistical weight factor of a level, E_{ji} is the transition energy.

Fe IV, N_f (E1 same-spin) = 14 145					
$N_i - N_j$	$T_iC_i - T_jC_j$	$g_i - g_j$	E_{ij}(Å)	S	AE1(s^{-1})
34–85	6De 2–6Fo 3	2–2	1663	2.55E-01	6.16E+08
35–85	6De 2–6Fo 3	4–2	1668	3.72E-02	1.78E+08
34–86	6De 2–6Fo 3	2–4	1657	2.01E-01	2.44E+08
35–86	6De 2–6Fo 3	4–4	1662	1.89E-01	4.55E+08
36–86	6De 2–6Fo 3	6–4	1669	2.73E-02	9.82E+07
35–87	6De 2–6Fo 3	4–6	1652	2.32E-01	3.77E+08
36–87	6De 2–6Fo 3	6–6	1660	1.56E-01	3.78E+08
37–87	6De 2–6Fo 3	8–6	1669	1.51E-02	4.82E+07
36–88	6De 2–6Fo 3	6–8	1647	2.77E-01	5.11E+08
37–88	6De 2–6Fo 3	8–8	1656	1.18E-01	2.86E+08
38–88	6De 2–6Fo 3	10–8	1668	5.44E-03	1.63E+07
37–89	6De 2–6Fo 3	8–10	1640	3.34E-01	6.62E+08
38–89	6De 2–6Fo 3	10–10	1651	6.71E-02	1.64E+08
38–90	6De 2–6Fo 3	10–12	1631	4.04E-01	8.45E+08
1–91	6Se 1–6Po 3	6–4	526	9.63E-02	3.47E+09
34–91	6De 2–6Po 3	2–4	1609	1.88E-01	2.42E+08
35–91	6De 2–6Po 3	4–4	1614	1.42E-01	3.63E+08
36–91	6De 2–6Po 3	6–4	1620	7.16E-02	2.73E+08
1–92	6Se 1–6Po 3	6–6	526	1.44E-01	3.47E+09
35–92	6De 2–6Po 3	4–6	1610	5.27E-02	9.03E+07
36–92	6De 2–6Po 3	6–6	1617	1.17E-01	2.99E+08
37–92	6De 2–6Po 3	8–6	1626	1.42E-01	4.77E+08
1–93	6Se 1–6Po 3	6–8	525	1.92E-01	3.48E+09
36–93	6De 2–6Po 3	6–8	1612	1.35E-02	2.60E+07
37–93	6De 2–6Po 3	8–8	1621	6.63E-02	1.68E+08
38–93	6De 2–6Po 3	10–8	1632	2.13E-01	6.65E+08
34–94	6De 2–6Do 3	2–2	1530	3.97E-02	1.13E+08
35–94	6De 2–6Do 3	4–2	1534	6.83E-02	3.87E+08
34–95	6De 2–6Do 3	2–4	1526	2.10E-01	3.01E+08
...	...	...	...	...	...
Fe IV, N_f (E1 intercombination+same-spin with $\Delta L = \pm 2$) = 30 691					
$N_i - N_j$	$T_iC_i - T_jC_j$	$g_i - g_j$	E_{ij}(Å)	S	AE1(s^{-1})
7–85	4Pe 1–6Fo 3	4–2	655	1.11E-06	3.44E+04
8–85	4Pe 1–6Fo 3	2–2	655	2.00E-06	3.10E+04
10–85	4De 1–6Fo 3	2–2	671	4.61E-06	6.82E+04
11–85	4De 1–6Fo 3	4–2	671	3.72E-06	1.10E+05
16–85	2De 1–6Fo 3	4–2	725	2.45E-06	6.20E+04
21–85	4Fe 1–6Fo 3	4–2	740	1.90E-05	4.62E+05
29–85	2Se 1–6Fo 3	2–2	825	8.38E-09	8.21E+01
30–85	2De 1–6Fo 3	4–2	878	5.70E-10	9.84E+00
39–85	2Pe 1–6Fo 3	4–2	1139	3.08E-09	3.16E+01
40–85	2Pe 1–6Fo 3	2–2	1139	8.68E-09	4.46E+01
42–85	2De 1–6Fo 3	4–2	1255	1.98E-08	1.67E+02
43–85	4De 2–6Fo 3	2–2	1992	1.08E-04	1.81E+05
44–85	4De 2–6Fo 3	4–2	2002	4.36E-05	1.45E+05
51–85	4Pe 2–6Fo 3	2–2	2921	1.96E-07	1.53E+02
52–85	4Pe 2–6Fo 3	4–2	2993	1.52E-09	2.26E+00
53–85	4Fe 2–6Fo 3	4–2	3137	1.51E-06	2.05E+03
64–85	2Pe 2–6Fo 3	2–2	3589	1.71E-08	8.88E+00
65–85	2Pe 2–6Fo 3	4–2	3800	5.23E-09	4.83E+00
74–85	4De 2–6Fo 3	4–2	4513	3.70E-07	2.42E+02
75–85	4De 2–6Fo 3	2–2	4529	7.20E-07	2.34E+02
80–85	2Se 2–6Fo 3	2–2	5830	1.21E-09	2.37E-01
1–86	6Se 1–6Fo 3	6–4	531	9.60E-08	3.40E+03
2–86	4Ge 1–6Fo 3	6–4	641	9.06E-06	2.20E+05
6–86	4Pe 1–6Fo 3	6–4	654	1.12E-06	2.62E+04
7–86	4Pe 1–6Fo 3	4–4	654	3.07E-06	4.78E+04
8–86	4Pe 1–6Fo 3	2–4	654	7.51E-07	5.84E+03
10–86	4De 1–6Fo 3	2–4	670	2.91E-07	2.16E+03
11–86	4De 1–6Fo 3	4–4	670	7.67E-06	1.14E+05
12–86	4De 1–6Fo 3	6–4	670	4.90E-06	1.09E+05
15–86	2Fe 1–6Fo 3	6–4	735	5.01E-07	9.26E+03
16–86	2De 1–6Fo 3	4–4	724	1.43E-08	1.81E+02
18–86	4Fe 1–6Fo 3	6–4	739	1.88E-05	3.44E+05
21–86	4Fe 1–6Fo 3	4–4	739	6.68E-08	8.14E+02
22–86	2De 1–6Fo 3	6–4	721	8.36E-06	1.61E+05
27–86	2Fe 1–6Fo 3	6–4	787	6.21E-08	1.00E+03
29–86	2Se 1–6Fo 3	2–4	823	4.78E-09	2.35E+01
30–86	2De 1–6Fo 3	4–4	877	2.43E-11	2.11E-01
31–86	2De 1–6Fo 3	6–4	877	3.36E-10	4.37E+00
39–86	2Pe 1–6Fo 3	4–4	1136	5.00E-08	2.58E+02
40–86	2Pe 1–6Fo 3	2–4	1136	1.84E-07	4.74E+02
...	...	...	...	...	...

Table 2. continued.

Fe IV, $N_f(E2) = 53201$, $N_f(M1) = 35\,667$					
$N_i - N_j$	$T_iC_i - T_iC_j$	$g_i - g_j$	E_{ij}(Å)	AE2(s^{-1})	AM1(s^{-1})
1–2	6Se 1–4Ge 1	6–6	3095	7.64E-09	2.16E-06
1–3	6Se 1–4Ge 1	6–8	3095	1.19E-08	8.29E-09
1–5	6Se 1–4Ge 1	6–10	3096	3.06E-10	0.00E+00
1–6	6Se 1–4Pe 1	6–6	2836	6.28E-05	1.21E+00
2–6	4Ge 1–4Pe 1	6–6	33863	2.41E-09	2.31E-05
3–6	4Ge 1–4Pe 1	8–6	33913	6.12E-09	3.57E-06
5–6	4Ge 1–4Pe 1	10–6	33763	9.14E-11	0.00E+00
1–7	6Se 1–4Pe 1	6–4	2830	3.52E-05	7.92E-01
2–7	4Ge 1–4Pe 1	6–4	32981	3.54E-09	3.26E-06
3–7	4Ge 1–4Pe 1	8–4	33028	1.65E-12	0.00E+00
1–8	6Se 1–4Pe 1	6–2	2824	7.11E-06	0.00E+00
2–8	4Ge 1–4Pe 1	6–2	32200	1.72E-10	0.00E+00
6–8	4Pe 1–4Pe 1	6–2	655597	1.27E-13	0.00E+00
1–9	6Se 1–4De 1	6–8	2578	1.22E-03	3.33E-04
2–9	4Ge 1–4De 1	6–8	15437	1.24E-07	5.15E-05
3–9	4Ge 1–4De 1	8–8	15447	1.55E-06	4.82E-04
4–9	4Ge 1–4De 1	12–8	15305	7.11E-07	0.00E+00
5–9	4Ge 1–4De 1	10–8	15416	4.78E-06	4.08E-04
6–9	4Pe 1–4De 1	6–8	28370	9.27E-06	5.45E-02
7–9	4Pe 1–4De 1	4–8	29021	5.73E-06	0.00E+00
1–10	6Se 1–4De 1	6–2	2570	2.00E-04	0.00E+00
2–10	4Ge 1–4De 1	6–2	15162	1.47E-06	0.00E+00
6–10	4Pe 1–4De 1	6–2	27456	2.22E-06	0.00E+00
7–10	4Pe 1–4De 1	4–2	28064	1.47E-05	5.10E-02
8–10	4Pe 1–4De 1	2–2	28656	0.00E+00	8.72E-02
1–11	6Se 1–4De 1	6–4	2568	6.80E-04	3.56E-02
2–11	4Ge 1–4De 1	6–4	15067	3.59E-06	1.53E-04
3–11	4Ge 1–4De 1	8–4	15077	1.41E-07	0.00E+00
6–11	4Pe 1–4De 1	6–4	27145	7.11E-06	2.55E-02
7–11	4Pe 1–4De 1	4–4	27740	6.50E-06	5.54E-02
8–11	4Pe 1–4De 1	2–4	28317	3.76E-06	2.27E-03
9–11	4De 1–4De 1	8–4	628459	9.15E-14	0.00E+00
1–12	6Se 1–4De 1	6–6	2568	1.15E-03	7.11E-02
2–12	4Ge 1–4De 1	6–6	15074	1.74E-06	3.90E-04
3–12	4Ge 1–4De 1	8–6	15084	4.47E-06	1.77E-07
5–12	4Ge 1–4De 1	10–6	15054	8.25E-08	0.00E+00
6–12	4Pe 1–4De 1	6–6	27169	1.07E-05	3.10E-02
7–12	4Pe 1–4De 1	4–6	27765	2.34E-07	5.02E-03
8–12	4Pe 1–4De 1	2–6	28344	6.15E-06	0.00E+00
9–12	4De 1–4De 1	8–6	641741	1.65E-13	1.10E-04
...	...	...	...	...	...
Fe IV, $N_f(E3) = 39\,423$					
$N_i - N_j$	$T_i\ C_i - T_i\ C_j$	$g_i - g_j$	E_{ij}(Å)	AE3(s^{-1})	
1–85	6Se 1–6Fo 3	6–2	532	6.52E-02	
2–85	4Ge 1–6Fo 3	6–2	642	1.34E-05	
3–85	4Ge 1–6Fo 3	8–2	642	1.88E-05	
6–85	4Pe 1–6Fo 3	6–2	655	2.58E-06	
9–85	4De 1–6Fo 3	8–2	670	1.50E-06	
12–85	4De 1–6Fo 3	6–2	671	6.74E-06	
15–85	2Fe 1–6Fo 3	6–2	736	3.17E-07	
17–85	2Fe 1–6Fo 3	8–2	732	6.75E-08	
18–85	4Fe 1–6Fo 3	6–2	740	5.92E-06	
20–85	4Fe 1–6Fo 3	8–2	739	4.10E-06	
22–85	2De 1–6Fo 3	6–2	722	3.03E-06	
25–85	2Ge 1–6Fo 3	8–2	766	7.65E-09	
27–85	2Fe 1–6Fo 3	6–2	789	3.78E-09	
28–85	2Fe 1–6Fo 3	8–2	789	2.51E-09	
31–85	2De 1–6Fo 3	6–2	879	4.61E-10	
33–85	2Ge 1–6Fo 3	8–2	952	2.94E-11	
36–85	6De 2–6Fo 3	6–2	1675	8.21E-04	
37–85	6De 2–6Fo 3	8–2	1685	1.35E-04	
41–85	2De 1–6Fo 3	6–2	1255	2.21E-10	
45–85	4De 2–6Fo 3	6–2	2018	1.01E-07	
46–85	4De 2–6Fo 3	8–2	2039	1.07E-08	
47–85	4He 2–6Fo 3	8–2	2967	1.66E-12	
54–85	4Fe 2–6Fo 3	6–2	3141	2.48E-10	
55–85	4Fe 2–6Fo 3	8–2	3148	1.87E-10	
56–85	4Pe 2–6Fo 3	6–2	3111	4.93E-09	
58–85	4Ge 2–6Fo 3	6–2	3430	1.72E-12	
59–85	4Ge 2–6Fo 3	8–2	3463	1.15E-12	
66–85	2Fe 2–6Fo 3	6–2	3874	6.43E-13	
67–85	2Fe 2–6Fo 3	8–2	3876	3.38E-13	
68–85	2Ge 2–6Fo 3	8–2	4360	1.59E-14	
72–85	4De 2–6Fo 3	8–2	4466	1.21E-12	
73–85	4De 2–6Fo 3	6–2	4488	2.47E-12	
77–85	2Ge 2–6Fo 3	8–2	4979	2.86E-17	
78–85	2De 2–6Fo 3	6–2	6046	4.40E-15	
...	...	...	...	...	...

should provide a more accurate distribution among fine structure components, especially for weaker and highly excited state transitions.

The present results also include same-spin transitions, but with $\Delta L = \pm 2$ which are possible through fine structure couplings. These transitions were not obtained in Nahar & Pradhan (2005). These together with intercombination transitions total 30 961 and complement the earlier set. Sample transitions are given in Table 2.

Fine structure transitions in Fe IV have been studied in relatively few investigations. Fawcett (1989) carried out earlier work for oscillator strengths for allowed E1 fine structure transitions using the semi-empirical method of Cowan (1968). The present same-spin and intercombination oscillator strengths agree well with those by Fawcett, especially for the stronger ones such as $a^6S_{5/2} - z^6P^\circ_{5/2}$ with no difference. However the difference can be considerable, especially for weaker ones such as for $a^4G_{9/2} - z^2H^\circ_{11/2}$ with an order of magnitude difference. A similar comparison was found between Fawcett and the earlier R-matrix results (Nahar & Pradhan 2005).

A and S values for 53 201 forbidden transitions of type E2 and 35 667 of type M1 for Fe IV are presented. Sample results from the complete set are given in Table 2. The decay rates of E2 and M1 transitions are compared in Table 3 with earlier rates obtained mainly among levels of the ground configuration, $3p^63d^5$. They were obtained by Garstang (1958, available in the evaluated compilation by the NIST at `www.nist.gov`), Raassen & Uylings (1996) using semi-empirical orthogonal operators (numbers are quoted in Froese Fischer & Rubin 2004), Froese Fischer & Rubin (1998, 2004) using a few approaches of relativistic multiconfiguration atomic structure calculations. A varying degree of agreement is found between the present results and the earlier works. For example, the present radiative rate for $^6S_{5/2} -^4 D_{3/2}$ agrees very well with that by Garstang (1958) as well as with the latest rate by Froese Fischer & Rubin (2004) while it is higher than the earlier value by Froese Fischer & Rubin (1998), However, the present result for $^6S_{5/2} -^4 P_{3/2}$ agrees much better with the earlier value of Froese Fischer and Rubin whereas it is lower than their latest rate. Garstang's earlier atomic structure calculations still agree well with all recent calculations for the lower fobidden transitions. Both the earlier and later calculations by Froese Fischer and Rubin focused considerably on optimization for the forbidden transitions among the levels of the ground configuration $3p^63d^5$ only, yet very large differences can be also be noticed in many transitions from their different approaches. All these discrepancies indicate that our results as well as those available in the literature are probably the best possible parameters that can be obtained at this time and a future attempt should be made with a larger set of configurations and with more computational resources. Experimental measurements are equally important and could be used to confirm various theoretical approaches.

The present results include transition probabilities for 39 423 electric octupole (E3) transitions. A sample set is presented in Table 2. No other data are available for comparison of these transitions.

Table 3. Comparison of present *A*-values for allowed and forbidden transitions in Fe IV with the available values: [r] R-matrix results (Nahar & Pradhan 2005), [s] Fawcett (1989), [a] NIST (Garstang 1958), [b] Froese Fischer & Rubin (2004), [c] Froese Fischer & Rubin (1998), [d] Raassen & Uylings (1996). [f] denotes oscillator strength comparison instead of *A*-values. The notation $n \pm y$ for a number means $n \times 10^{\pm y}$.

Present	Previous	$SL_i - SL_k$	$J_i - J_k$	Type
3.48+9	3.40+9[r]	a^6S – z^6P°	5/2–7/2	E1
3.47+9	3.38+9[r]	a^6S – z^6P°	5/2–3/2	E1
2.42+8	2.37+8[r]	a^6D – z^6P°	1/2–3/2	E1
6.16+8	5.50+8[r]	a^6D – z^6F°	1/2–1/2	E1
1.78+8	1.58+8[r]	a^6D – z^6F°	3/2–1/2	E1
4.55+8	4.03+8[r]	a^6D – z^6F°	3/2–3/2	E1
0.144	0.144[s]:f	a^6S – z^6P°	5/2–5/2	E1
0.0963	0.116[s]:f	a^6S – z^6P°	5/2–3/2	E1
0.0096	0.013[s]:f	a^4G – z^4F°	5/2–5/2	E1
0.0622	0.0668[s]:f	a^4G – z^4F°	5/2–3/2	E1
3.6-4	9.5-3[s]:f	a^4G – z^2H°	9/2–11/2	E1
4.5-4	1.17-3[s]:f	a^4G – z^2I°	11/2–13/2	E1
0.0464	0.0247[s]:f	a^4P – z^2F°	5/2–7/2	E1
3.56-2	3.8-2[a],3.33-2[b],1.65-2[c]	^{6}S –^{4} D	5/2–3/2	M1
7.11-2	5.1-2[a],6.64-2[b],3.4-2[c]	^{6}S –^{4} D	5/2–5/2	M1
0.792	0.88[a],1.02[b],0.759[c]	^{6}S –^{4} P	5/2–3/2	M1
1.21	1.4[a],1.56[b],1.17[c]	^{6}S –^{4} P	5/2–5/2	M1
3.52-5	1.21-5[b],1.99-5[d]	^{6}S –^{4} P	5/2–3/2	E2
6.28-5	4.0-05[b],4.26-5[d]	^{6}S –^{4} P	5/2–5/2	E2
1.19-8	3.32-8[b],3.18-8[d]	^{6}S –^{4} G	5/2–7/2	E2
7.64-9	2.3-8[b],1.95-8[d]	^{6}S –^{4} G	5/2–5/2	E2
2.31-5	6.8-5[a],1.32-4[b],7.90-5[c]	^{4}G –^{4} P	5/2–5/2	M1
3.57-6	1.5-5[a],2.37-5[b],1.51-5[c]	^{4}G –^{4} P	7/2–5/2	M1
6.12-9	3.68-9[b]3.42-9[d]	^{4}G –^{4} P	7/2–5/2	E2
2.31-9	1.86-9[b],1.83-9[d]	^{4}G –^{4} P	5/2–5/2	E2
8.72-2	5.8-2[a],7.07-2[b],4.94-2[c]	^{4}P –^{4} D	1/2–1/2	M1
5.45-2	3.8-2[a],4.56-2[b],3.31-2[c]	^{4}P –^{4} D	5/2–7/2	M1
5.15-5	7.6-5[a],1.33-4[b],8.18-5[c]	^{4}G –^{4} D	5/2–7/2	M1
0.661	0.72[a],0.824[b]	^{4}D –^{2} D2	7/2–5/2	M1
2.14-5	1.21-5[b]	^{4}D –^{2} D2	7/2–5/2	E2
0.14	0.16[a].0.257[b]	^{4}D –^{2} D2	5/2–5/2	M1
2.15-4	1.71-4[b]	^{4}D –^{2} D2	5/2–5/2	E2
0.25	0.027[a].0.333[b]	^{4}D –^{2} D2	3/2–5/2	M1
8.11-2	9.0-2[a],1.12-1[b]	^{4}D –^{2} D2	5/2–3/2	M1
1.56-4	5.7-5[b]	^{4}D –^{2} D2	5/2–3/2	E2
0.217	0.22[a],0.312[b]	^{4}D –^{2} D2	3/2–3/2	M1
1.91-5	1.84-5[b]	^{4}D –^{2} D2	3/2–3/2	E2
5.25-4	2.42-5[b]	^{4}D –^{2} D	3/2–3/2	E2
3.60-4	1.66-5[b]	^{4}D –^{2} D	3/2–3/2	M1
1.70-5	9.1-5[b]	^{4}P –^{2} S	5/2–1/2	M1
0.63	0.73[a],0.797[b]	^{4}P –^{2} S	3/2–1/2	M1
0.129	0.11[a],0.16[b]	^{4}P –^{2} S	1/2–1/2	M1
1.14-3	7.8-2[a],2.16-3[b]	^{4}D –^{2} S	1/2–1/2	M1
1.99-2	1.0-2[a],1.75-2[b]	^{4}D –^{2} S	3/2–1/2	M1
1.24-4	1.08-4[b]	^{4}D –^{2} S	3/2–1/2	E2
3.24-4	2.37-4[b]	^{4}D –^{2} S	5/2–1/2	E2
5.72	4.2[a]	^{2}I –^{2} G1	11/2–7/2	E2
0.176	0.12[a]	^{2}I –^{2} G1	11/2–9/2	E2
5.59	4.1[a]	^{2}I –^{2} G1	13/2–9/2	E2
0.132	0.18[a]	^{2}I –^{2} H	11/2–11/2	M1
7.06-2	9.4-2[a]	^{2}I –^{2} H	13/2–11/2	M1
0.547	0.40[a]0.46[b]	^{2}G2 –^{2} G1	7/2–7/2	E2
0.046	0.028[a],0.0335[b]	^{2}G2 – 2G1	9/2–7/2	M1
0.476	0.29[a].0.365[b]	^{2}G2 –^{2} G1	9/2–9/2	E2
3.10-2	6.4-2[a],3.95-2[b]	^{4}G –^{2} G2	7/2–9/2	M1
5.42-3	7.7-2[a],6.4-2[b]	^{4}G –^{2} G2	9/2–7/2	M1

Table 4. Comparison of present lifetimes (τ) in seconds with those by Kurucz (2005) for levels of Fe IV. The number within parentheses next to τ is the total number of present *A*-values included for transitions from that level.

Present	Kurucz	SL_J
4.48 (38)	4.83	$3d^5\ a^2F_{5/2}$
2.52-4 (52)	2.77-4	$3d^4 4s\ a^2I_{11/2}$
6.06-10 (64)	5.95-10	$3d^4 4p\ ^4P^\circ_{1/2}$
2.97-10 (95)	3.09-10	$3d^4 4p\ ^4D^\circ_{7/2}$

4.1. Lifetimes

The lifetime of a level can be obtained from the sum of the radiative decay rates of the level to various lower levels. The program LIFETMBP (with the electronic data files) can read the files for radiative decay rates and compute the lifetimes. Example lifetimes for Fe IV are given in Table 4. These lifetimes agree very well with those by Kurucz (2005).

5. Conclusion

An extensive set of about 173 000 radiative decay rates and line strengths for transitions in Fe IV are presented for various astrophysical applications. The transitions are of allowed E1, forbidden E2, E3 and M1 types and correspond to transitions among the closely lying 1275 levels of the ground and six excited configurations of Fe IV. It is important for a model to include all transitions of levels that lie close together, such as considered in the present work, as they cause blendings in the spectra. The relativistic effects have been included through the Breit-Pauli approximation in the code SUPERSTRUCTURE. The reprocessed *S* and *A* data with the observed energies are more appropriate for applications in astrophysical models as the latter use the available observed transition energies. The new results should be particularly useful for the analysis of optical Ultraviolet spectra from astrophysical and laboratory sources where non-local thermodynamic equilibrium (NLTE) atomic models with many excited levels are needed. The complete file of the present transitions and energy levels is available electronically.

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